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Thermochemistry of ammonium based ionic liquids: Thiocyanates - Experiments and computations

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Abstract

© Springer Science+Business Media New York 2015. Abstract Molar enthalpies of solution of tetra-n-butylammonium thiocyanate [N(Bu)4][SCN] and tetra-n-pentylammonium thiocyanate [N(Pe)4][SCN] in water were measured by using solution calorimetry. The enthalpy of combustion of [N(Bu)4][SCN] was measured by using rotation bomb combustion calorimetry and the enthalpy of formation of this ionic liquids was derived. The thermal behavior of [N(Bu)4][SCN] was studied using differential scanning calorimetry. Quantum-chemical calculations of the molar enthalpy of formation in the gaseous phase have been performed for the series [N(R)4][SCN] with RA =(Me, Et, n-Bu, and n-Pe) using the G3MP2 level of theory. Experimental and calculated values of the enthalpies of formation are in agreement within the boundaries of the experimental uncertainties.

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Keywords

Combustion calorimetry, Enthalpy of formation, Enthalpy of solution, Ionic liquids, Quantum-chemical calculations, Solution calorimetry